

4,4'-(Propane-2,2-diyl)di(²H₄)phenol
92739-58-7 | DTXSID40662328

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 15.1 days

Global applicability domain: Outside

Local applicability domain index: 2.88e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>9-Ethyl-9H-fluorene</div> <div>Measured: 2330</div> <div>Predicted: N/A</div>	<div>Image not found</div> <div>2-Methylphenanthrene</div> <div>Measured: 1370</div> <div>Predicted: 25.0</div>	<div>Image not found</div> <div>5-Methylindan</div> <div>Measured: 4.93</div> <div>Predicted: 2.25</div>
<div>Image not found</div> <div>4-Phenyltoluene</div> <div>Measured: 4340</div> <div>Predicted: 25.1</div>	<div>Image not found</div> <div>2-Methylnaphthalene</div> <div>Measured: 436</div> <div>Predicted: 15.3</div>	